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14. ABSTRACT

The overall goal of the research was to advance capabilities for the computational modeling of turbulent combustion. The design of combustors in propulsion systems for space and aircraft applications remains a significant technical challenge, and computational modeling is used extensively in the design process. Significant progress was made in four areas. A storage/retrieval methodology for the efficient implementation of combustion chemistry was extended for use on parallel clusters. Based on the solution of a modeled transport equation for the joint probability density function, calculations were performed of lifted hydrogen flames in vitiated co-flows. These revealed that the stabilization mechanism was lateral mixing followed by autoignition; and that the flame lift-off height is extremely sensitive to the co-flow temperature. Similar calculations were performed for methane/air piloted jet flames using mechanisms with up to 53 chemical species. These computations demonstrated the level of description of the chemistry needed for the accurate calculation of the finite-rate chemical effects in these flames. A new dimension-reduction methodology was developed and demonstrated which reduces the computational cost of incorporating realistic combustion chemistry. In addition, there were collaborations with the University of Pittsburgh and Clemson University on large-eddy simulations of turbulent combustion using probability density function methods.

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PDF MODELLING OF TURBULENT COMBUSTION

AFOSR Grant F-49620-03-1-0015
Principal Investigator: Stephen B. Pope
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FINAL TECHNICAL REPORT
1/12/2002 – 8/31/2005

ABSTRACT

The overall goal of the research was to advance capabilities for the computational modeling of turbulent combustion. The design of combustors in propulsion systems for space and aircraft applications remains a significant technical challenge, and computational modeling is used extensively in the design process. Significant progress was made in four areas. A storage/retrieval methodology for the efficient implementation of combustion chemistry was extended for use on parallel clusters. Based on the solution of a modeled transport equation for the joint probability density function, calculations were performed of lifted hydrogen flames in vitiated co-flows. These revealed that the stabilization mechanism was lateral mixing followed by autoignition; and that the flame lift-off height is extremely sensitive to the co-flow temperature. Similar calculations were performed for methane/air piloted jet flames using mechanisms with up to 53 chemical species. These computations demonstrated the level of description of the chemistry needed for the accurate calculation of the finite-rate chemical effects in these flames. A new dimension-reduction methodology was developed and demonstrated which reduces the computational cost of incorporating realistic combustion chemistry. In addition, there were collaborations with the University of Pittsburgh and Clemson University on large-eddy simulations of turbulent combustion using probability density function methods.

EXECUTIVE SUMMARY

The overall goal of the research was to develop and demonstrate improved computational approaches for turbulent combustion. In both space and aircraft applications, the design of combustors in propulsion systems remains a significant technical challenge; and computational modeling is used extensively in the design process. Our work was aimed at increasing the accuracy and efficiency of such models. In the reporting period the research has focused on four topics which are summarized here, and described more fully in the following four sections.

The first topic is the use of *in situ* adaptive tabulation (ISAT) on parallel clusters. In most approaches to computing combustion with realistic chemical kinetics, the computational

bottleneck is associated with computing the effect of chemical reactions on the fluid composition. The ISAT algorithm (Pope 1997) has been shown to be effective in speeding up this process, typically by two or three orders of magnitude. The research performed here is to devise and investigate different strategies for implementing ISAT on parallel computers. The work, which is on-going, is described in Lu et al. (2004, 2005).

The second topic is the calculation of lifted hydrogen jet flames in vitiated co-flows. Two studies have been performed, the first (Masri et al. 2004) based on the composition PDF method incorporated in the Fluent CFD code; the second (Cao et al. 2005) based on the joint PDF of velocity, frequency and composition. In both cases the calculations are compared to the experimental data of Cabra et al. (2002). These studies: reveal the stabilization mechanism of these flames; show the extreme sensitivity of the lift-off height to the co-flow temperature; show the relative sensitivity of the calculations to the chemical kinetics; and show the relative insensitivity to the modeling of turbulent mixing.

The third topic is the study of piloted methane/air jet flames (Barlow & Frank 1998) through computations based on the modeled equation for the joint PDF of velocity turbulence frequency and composition. These calculations (Cao & Pope 2005) compare the performance of seven different chemical mechanisms for methane combustion. It is found that accurate calculations are possible with detailed mechanisms (e.g., GRI 3.0 which contains 53 species), and also with augmented reduced mechanisms. (e.g., with of order 20 species). On the other hand, the simpler mechanisms examined (e.g., C_1 skeletal mechanisms and 5-step reduced mechanisms) are inaccurate.

The fourth topic concerns the dimension reduction of combustion chemistry. In previous work Tang & Pope (2002) developed and demonstrated a dimension reduction technique (rate-controlled constrained equilibrium, RCCE, Keck & Gillespie 1971) coupled with ISAT. In the current work (Tang & Pope 2003) it is shown how the accuracy of the dimension reduction can be significantly improved.

In addition to these four topics studied at Cornell, the PI has collaborated with Professor Peyman Givi's group at the University of Pittsburgh, and with Professor Chenning Tong's group at Clemson University. The resulting publications are Sheikhi et al. (2003, 2005) and Wang et al. (2004).

EFFICIENT PARALLEL IMPLEMENTATION OF IN SITU ADAPTIVE TABULATION

The PDF method calculations presented below demonstrate current capabilities, e.g., using a mechanism with of order 50 species. Such calculations are possible because of the ISAT algorithm and the availability of parallel computers. As we work towards combining PDF methods with large eddy simulation (LES), larger parallel clusters are needed, and the efficient parallel implementation of ISAT becomes critical.

If there are P processors, then the load associated with solving the LES equations is well balanced if the solution domain is partitioned into P subdomains, each containing

approximately the same number of computational cells. Further, with such a decomposition, the computational particles used in the PDF algorithm are approximately equally distributed between the processors. Hence there is good load balancing of particle tracking and of mixing. However, the load associated with reaction (i.e., incrementing the particle compositions due to reaction over the time step) which can dominate the CPU time can be poorly balanced. For example, the particles on one processor may be inert (e.g., cold air) and hence require negligible time to evaluate their reaction; whereas the particles on another processor may be highly reactive. Even using ISAT, reactive particles take much longer to treat, especially if retrieving from a full table is not possible, and hence a direct integration of the stiff ordinary differential equations is required.

In the work described by Lu et al. (2005) we have implemented and evaluated three strategies, in each of which, each of the P processors maintain its own (independent) ISAT table. In the first, referred to as LOCAL, there is no message passing: each processor evaluates reaction for all of its resident particles using its own ISAT table. This LOCAL strategy obviously minimizes message passing, but does nothing to remedy load imbalances. In the second, referred to as URAN, each particle is randomly assigned to one of the P processors with equal probability. The particle is passed to the assigned processor, ISAT is used to evaluate the effects of reaction, and the particle is passed back. This URAN strategy creates a great deal of message passing, but guarantees load balancing. However, the total "load" depends on how ISAT is employed, so load balancing alone is not necessarily optimal. In the third strategy, referred to as STRATA, the particles are stratified (i.e., binned according to their value of mixture fraction), and each processor handles all particles in a particular mixture-fraction range. As a consequence, each ISAT table is required to tabulate just a fraction (roughly $1/P$) of the composition space.

The relative merits of the three strategies depend on several parameters–the complexity of the chemistry, the length of the simulation, the number of processors, etc. Figure 1 demonstrates the performance for a test case of a 2D LES/PDF calculation of a methane/air mixing layer, using a 35-species mechanism (GRI 3.0 without NO chemistry). For each of the 8 processors used, the figure shows the average wall clock and CPU times required per LES/PDF time step to perform reaction. As may be seen, LOCAL exhibits considerable load imbalance. For URAN the load is extremely well balanced, but nevertheless it is outperformed by STRATA. An improved stratification strategy can be expected to achieve improved load balance, and even better performance.

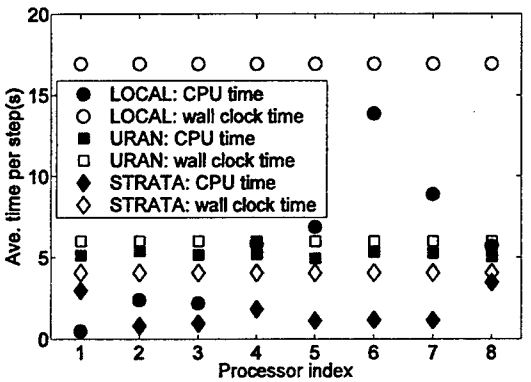

Fig. 1. Average wall-clock and CPU times required for the reaction fraction step in an LES/PDF calculation of a methane/air mixing layer using different ISAT parallel strategies.

PDF CALCULATIONS OF LIFTED TURBULENT FLAMES

In laboratory experiments on turbulent flames, for obvious reasons, air at atmospheric conditions is generally used as the oxidant. In practical applications, however, the re-circulating flows used for flame stabilization generally lead to some mixing between the air stream and hot combustion products. In thrust augmentors the oxidant stream is simply the lean combustion products from the turbine.

Motivated by this observation, a series of experiments has been performed (at the University of California, Berkeley; Sandia National Laboratories; and the University of Sydney) on various jet flames in vitiated co-flows. Two PDF studies have been performed of the lifted hydrogen flames studied experimentally by Cabra et al. (2002). These two studies are based on the composition PDF method incorporated in Fluent (Masri et al. 2004), and on the velocity-frequency-composition joint PDF method (Cao, Pope & Masri 2005). In both cases, detailed 9-species mechanisms for hydrogen are used. The principal findings are:

1. The PDF calculations are successful in reproducing the observed dependence of lift-off height on the temperature of the vitiated co-flow.
2. The calculations clearly show that the base of the flame is controlled by the autoignition of very lean mixtures.
3. The calculations exhibit a sensitivity to the chemical mechanism employed but much less sensitivity to the mixing model.

This last conclusion is substantiated by the results presented in Fig. 2, which show the lift-off height calculated using two different chemical mechanisms and three different turbulent mixing models. It should be noted that all the calculations are well within the horizontal experimental error bars (not shown), which correspond to an uncertainty in the co-flow temperature of ± 25 K.

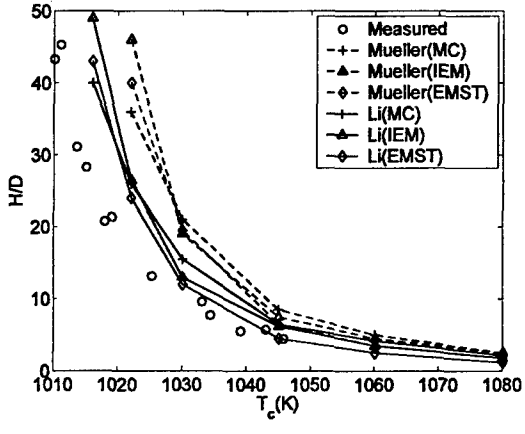

Fig. 2: Lift-off height against co-flow temperature. Circles, experimental data of Wu et al. (2003); lines, PDF calculations with the Mueller and Li mechanisms, and with the modified Curl (MC), interaction by exchange with the mean (IEM) and Euclidean minimum spanning tree (EMST) mixing models. (From Cao, Pope & Masri, 2005.)

An important outstanding question is the accuracy of the mixing sub-models used in PDF models. The three most widely used models are named interaction by exchange with the mean (IEM), modified Curl (MC) and Euclidean minimum spanning tree (EMST). It has been found previously that, in some circumstances, these three models yield significantly

different results (Subramaniam & Pope 1999, Ren & Pope 2004). For the lifted hydrogen flame in a vitiated co-flow, Fig. 3 shows the lift-off height as a function of the co-flow temperature for the three mixing models. The sensitivity to the choice of model is not great. It remains to delineate the circumstances in which the different models provide an adequate description of mixing.

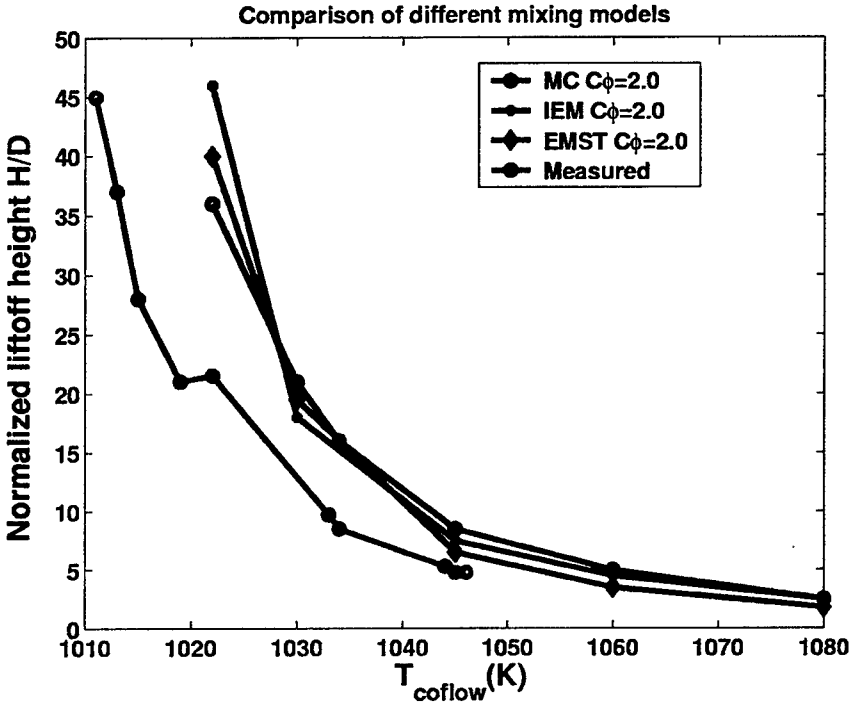

Figure 3. Lift-off height (in jet diameters) against co-flow temperature for the hydrogen jet flame in a vitiated co-flow: comparison of experimental measurements and joint PDF calculations with three different mixing models.

PDF CALCULATIONS OF PILOTED JET FLAMES

The Barlow & Frank (1998) piloted jet flames are well recognized as providing an excellent test of turbulent combustion models, in particular of their ability to describe local extinction and re-ignition. There is a sequence of flames *A*–*F*, with *D*, *E* and *F* being fully turbulent, with increasing amounts of local extinction. While there are many successful modeling studies of flame *D*–which has little local extinction–there are far fewer of the more challenging flames *E* and *F*.

PDF methods have previously been applied successfully to these flames by Xu & Pope (2000), Tang et al. (2000), and Lindstedt et al. (2000). Since the Cornell and Imperial College groups use different mixing models and different chemical mechanisms, questions arise as to the dependence and sensitivity of the calculations to these ingredients. Some progress has been made in understanding the relative behavior of the different mixing models (see, e.g., Ren & Pope 2004). Very recently, we (Cao & Pope 2005) have

performed joint PDF calculations of these flames using 6 different chemical mechanisms for methane, ranging from a 5-step reduced mechanism, to the 53-species GRI 3.0 mechanism. As an example of the results obtained, Fig. 4, shows a comparison of the conditional mean temperature (conditional on mixture fraction) in flame F at an axial difference of 15 nozzle diameters (the location of maximum local extinction). The 5-step reduced mechanism (S5G211) substantially underestimates the amount of local extinction, whereas the other four mechanisms yield approximately the experimentally-observed values. The sixth mechanism considered (a 16-species C_1 mechanism, Smooke et al. 1986) predicts global extinction.

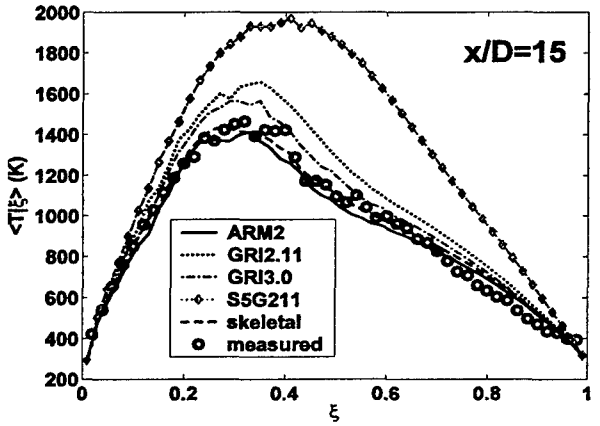

Fig. 4: Conditional mean temperature at x/D = 15 in flame F: measurements of Barlow & Frank (1998); joint PDF calculations with different chemical mechanisms of Cao & Pope (2005).

DIMENSION REDUCTION OF COMBUSTION CHEMISTRY

In the past two decades, one of the most important triumphs in combustion research is the numerical simulation of laminar flames in one or two spatial dimensions, taking account of detailed transport and chemical kinetics. However, for most practical reacting flows featuring three dimensional geometric complexity and turbulence, a detailed numerical simulation will remain computationally prohibitive, even on the largest supercomputers. To make calculations of turbulent combustion with realistic chemistry feasible, it is necessary to reduce the computational cost of solving the complex thermo-chemical system.

The work of Tang and Pope (2002) describes a unified dimension reduction/storage retrieval methodology which can be used to implement detailed hydrocarbon chemistry efficiently in turbulent combustion calculations. Dimension reduction is achieved through rate-controlled constrained equilibrium (RCCE) (Keck & Gillespie 1971), and storage/retrieval through *in situ* adaptive tabulation (ISAT). In this context, RCCE is preferred over other reduction methodologies, such as quasi-steady state assumption (QSSA) and intrinsic low-dimensional manifold (ILDM) (Maas & Pope 1992), because of the guaranteed existence and smoothness of the implied low-dimensional constrained equilibrium manifold (CEM). However, RCCE is based solely in thermodynamics, whereas QSSA and ILDM are based appropriately on dynamical-systems approaches to the chemical kinetics. RCCE's "efficiency" is questionable, therefore, since it is not clear that the implied reduction assumptions are near optimal.

In this study, an orthogonal projection contained in the traditional RCCE method, which projects the rate equation of the chemical system onto the constrained equilibrium manifold, is identified. A more accurate projection, which we refer to as the close parallel inertial manifold (CPIM) then is constructed. The CPIM assumption introduces the chemical kinetics directly through the local Jacobian of the chemically reacting system and hence leads to greater accuracy than RCCE.

As an illustration of the methodology, Fig. 5 shows calculations for the autoignition of a methane-air mixture initially at 1500K. The CPIM results are almost indistinguishable from those from the detailed mechanism, while RCCE overpredicts the ignition delay time by about a factor of two.

In more recent work (under other funding) an improved dimension reduction methodology has been developed (Ren et al. 2006a, b). Interestingly, the CPIM concept plays a central role in the newer methodology.

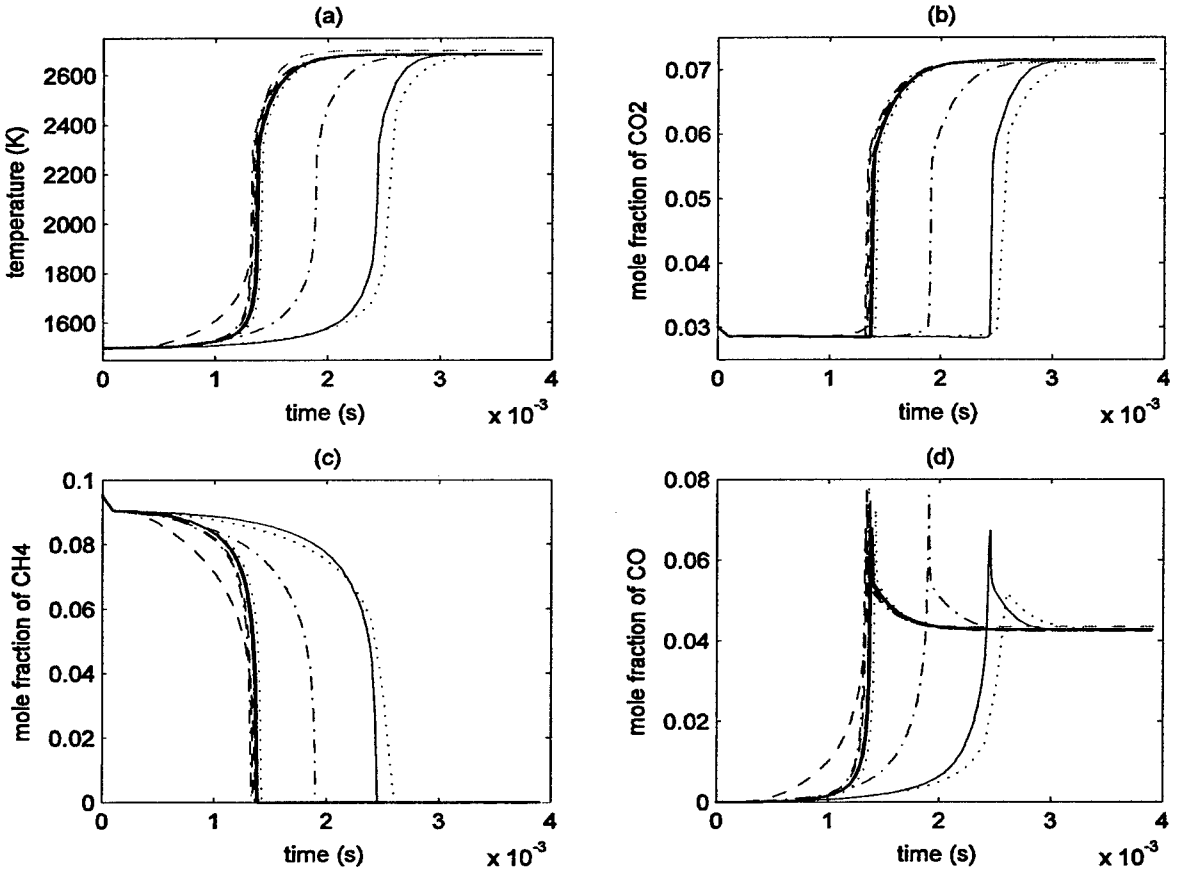

Figure 5: Comparisons of major species mole fractions against time calculated using RCCE and CPIM (T_0 = 1500 K, p = 1 atm, and Φ =1). Black: exact solution; Red: CPIM; Blue: RCCE.

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PERSONNEL SUPPORTED

Prof. S.B. Pope, PI
Prof. A.R. Masri, sabbatical visitor
Qing Tang, Ph.D. student
Renfeng Cao, Ph.D. student
Andrea Lamorgese, Ph.D. student
Liuyan Lu, Ph.D. student
Darius Liu, undergraduate student, then M.S. student

DEGREES GRANTED

Qing Tang, Ph.D., May 2003
Darius Liu, M.S., August 2004
Renfeng Cao, Ph.D., August 2005

MEETING PARTICIPATION

March 16-19, 2003: Third Joint Meeting of the U.S. Sections of the Combustion Institute. Three contributed papers and posters. Chicago, IL.

May 25-30, 2003: Computation Fluid Dynamics in Chemical Reaction Engineering III. Invited lecture. Davos, Switzerland.

June 23-25, 2003: ARO/AFOSR Contractors' Meeting in Chemical Propulsion. Williamsburg, VA.

July 18-19, 2003: Fête Antonia. Invited talk. Newcastle, Australia.

July 21-23, 2003: TNF7 Planning Meeting, Sydney, Australia.

October 26-29, 2003: Eastern States Meeting of the Combustion Institute, Penn. State University.

November 23-25, 2003: American Physical Society, Meadowlands, NJ.

December 8-9, 2003: Workshop on LES & SGS Modelling for Turbulent Mixing and Reactive Flows, Caltech, invited talk.

May 17-21, July 14-16, 2004: Stanford/Ames CTR Summer Program.

June 1-3, 2004: Doe Contractors' Meeting, Warrenton, VA.

June 7-9, 2004: ARO/AFOSR Contractors' Meeting, Tuscon, AZ.

June 23-24, 2004: Computing the Future, Cornell University.

June 29-July 2, 2004: Tenth European Turbulence Conference, Trondheim, Norway (invited plenary lecture).

July 22-24, 2004: TNF7, Seventh International Workshop on Measurements and Computations of Nonpremixed Turbulent Flames, Chicago IL.

July 26-30, 2004: 30th International Combustion Symposium, Chicago, IL.

November 22, 2004: American Physical Society, Division of Fluid Dynamics, Annual Meeting, Seattle, invited talk in session honoring Bill Reynolds and two contributed talks.

March 20-23, 2005: Joint Meeting of the U.S. Sections of the Combustion Institute, Drexel University, Philadelphia, Organized session on LES/FDF modeling of turbulent combustion.

The Merck Lecture, Chemical Engineering, Rutgers University, NJ.

June 1-3, 2005: DOE Contractors' Meeting, Warrenton, VA

June 20-22, 2005: ARO/AFOSR Contractors' meeting, Indianapolis, IN.

INTERACTION WITH AFRL

On June 24, 2003, during the AFO/AFOSR contractors meeting in Williamsburg, VA, Dr. Joesph Zelina and I discussed his use of CFD for the Ultra-Compact Combustor (UCC). Currently CFD calculations are being performed using Fluent with standard turbulence and combustion models. The available experimental data are at present insufficient to assess the quality of these calculations. It is possible that in the future additional personnel may be available to perform more extensive calculations. These could include PDF model computations (using Fluent) to explore in more detail the compositional fields in the UCC.

On June 8, 2004, in Tucson, Arizona, during the ARO/AFOSR Contractors' Meeting, I discussed with Joseph Zelina the current CFD and turbulent combustion modeling activities at AFRL. In a follow-up phone call on August 3, it was agreed that it would be valuable for me to discuss combustion modeling issues with Vish Katta of ISSI. In the subsequent conversation with Vish Katta we discussed (a) the possible use of his data in research at Cornell to investigate the dimensionality of combustion chemistry, and (b) the possible use of a storage/retrieval algorithm such as ISAT in Katta's calculations. It appears that this would not be beneficial because the computation of molecular transport (not of reaction) is the dominant cost.

At the ARO/AFOSR Contractors' Meeting (June 20-22, 2005 in Indianapolis) the PI had conversations with Joe Zelina concerning the CFD activities at AFRL. Of particular current interest is the performance of model calculations of inter-turbine burning (ITB). The code being used is ACE, from CFDRC, which includes RANS, LES and PDF capabilities, as well as ISAT. This activity is likely to increase as Capt. Roger Greenwood denotes more time to it, and the PI has offered to assist as appropriate.

TECHNOLOGY TRANSITIONS AND TRANSFERS

The computer program implementing the EMST mixing model has been re-written to make it more easily useable by others, and it has been made openly available on the web (http://mae.cornell.edu/~laniu/emst). This mixing model is arguably the best available for use in PDF methods for turbulent combustion. It was developed by S. Subramaniam and S.B. Pope with previous AFOSR support. Using these routines, Dr. Graham Goldin of Fluent, Inc. has implemented the EMST mixing model into the commercial CFD code, Fluent 6.2.

Performer	Customer	Result	Application
Dr. S.B. Pope Cornell Univ. (607) 255-4314	Dr. Graham Goldin Fluent, Inc. Lebanon, NH (603) 643-2600	Computer program implementing the EMST mixing model	Fluent application in the design of combustion devices

HONORS AND AWARDS

Elected Fellow of the Institute of Physics
Elected Vice-Chair of the American Physical Society, Division of Fluid Dynamics (to serve as Chair elect and Chair in 2005-06 and 2006-07).

INVENTIONS AND PATENTS

There were no inventions or patents during the reporting period.

PUBLICATIONS

The following papers were written and/or published during the reporting period.

Q. Tang and S.B. Pope (2002) "Implementation of combustion chemistry by *in situ* adaptive tabulation of rate-controlled constrained equilibrium manifolds," Proc. Comb. Inst. **29**, 1411-1417.

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Q. Tang and S.B. Pope (2004) "A more accurate projection in the rate-controlled constrained-equilibrium method for dimension reduction of combustion chemistry", Combustion Theory and Modelling **8**, 255-279.

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